

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF100724\  
 Data File : BF139689.D  
 Acq On : 07 Oct 2024 16:33  
 Operator : RC/JU  
 Sample : P4274-01  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 222254

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139689.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 2.163       | 3             | 12          | 18           | rBV      | 4900073        | 9076269       | 100.00%         | 35.123%       |
| 2         | 5.487       | 571           | 577         | 587          | rBV      | 971294         | 1260547       | 13.89%          | 4.878%        |
| 3         | 6.492       | 743           | 748         | 761          | rVB      | 636179         | 800480        | 8.82%           | 3.098%        |
| 4         | 6.863       | 806           | 811         | 816          | rBV      | 424943         | 512378        | 5.65%           | 1.983%        |
| 5         | 7.428       | 900           | 907         | 912          | rBV      | 1413414        | 1904121       | 20.98%          | 7.369%        |
| 6         | 8.145       | 1021          | 1029        | 1034         | rBV      | 539455         | 663651        | 7.31%           | 2.568%        |
| 7         | 9.222       | 1206          | 1212        | 1217         | rBV      | 2523462        | 3257378       | 35.89%          | 12.605%       |
| 8         | 9.898       | 1322          | 1327        | 1336         | rVB      | 608427         | 770921        | 8.49%           | 2.983%        |
| 9         | 10.616      | 1443          | 1449        | 1455         | rBV      | 66366          | 92895         | 1.02%           | 0.359%        |
| 10        | 10.692      | 1456          | 1462        | 1470         | rBV      | 1562431        | 2090954       | 23.04%          | 8.092%        |
| 11        | 11.386      | 1575          | 1580        | 1585         | rBV      | 682596         | 838318        | 9.24%           | 3.244%        |
| 12        | 11.910      | 1661          | 1669        | 1687         | rBV3     | 99712          | 214626        | 2.36%           | 0.831%        |
| 13        | 12.974      | 1844          | 1850        | 1855         | rBV      | 2507483        | 3314350       | 36.52%          | 12.826%       |
| 14        | 14.027      | 2023          | 2029        | 2035         | rBV      | 458515         | 600874        | 6.62%           | 2.325%        |
| 15        | 15.498      | 2273          | 2279        | 2290         | rBV      | 284347         | 443524        | 4.89%           | 1.716%        |

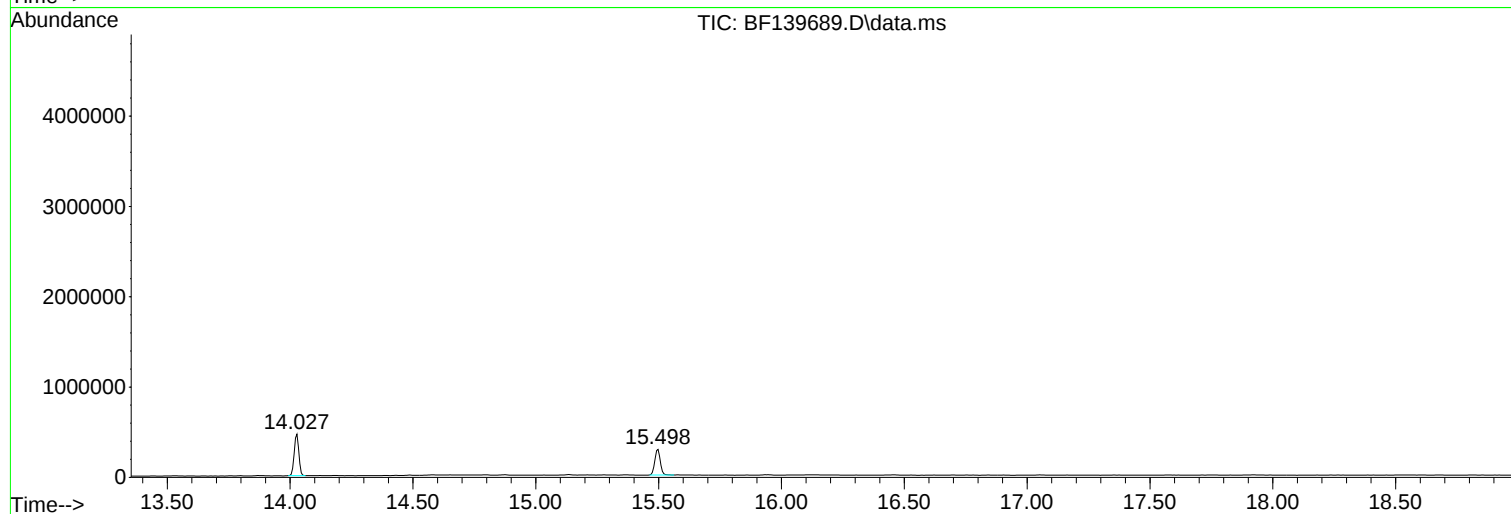
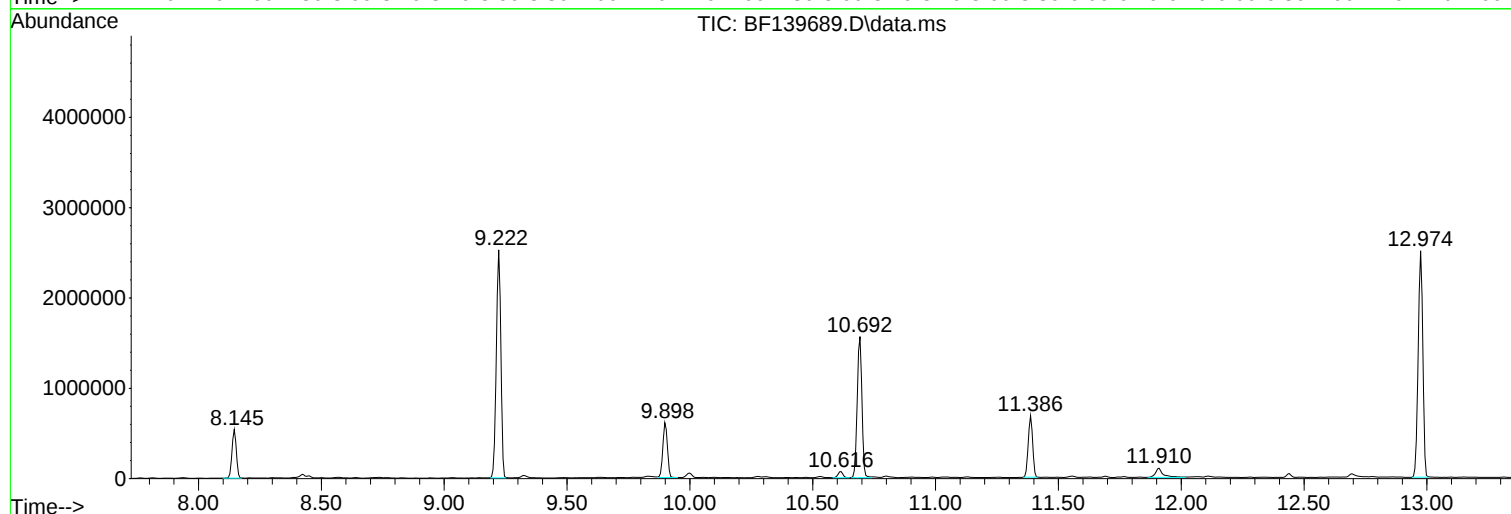
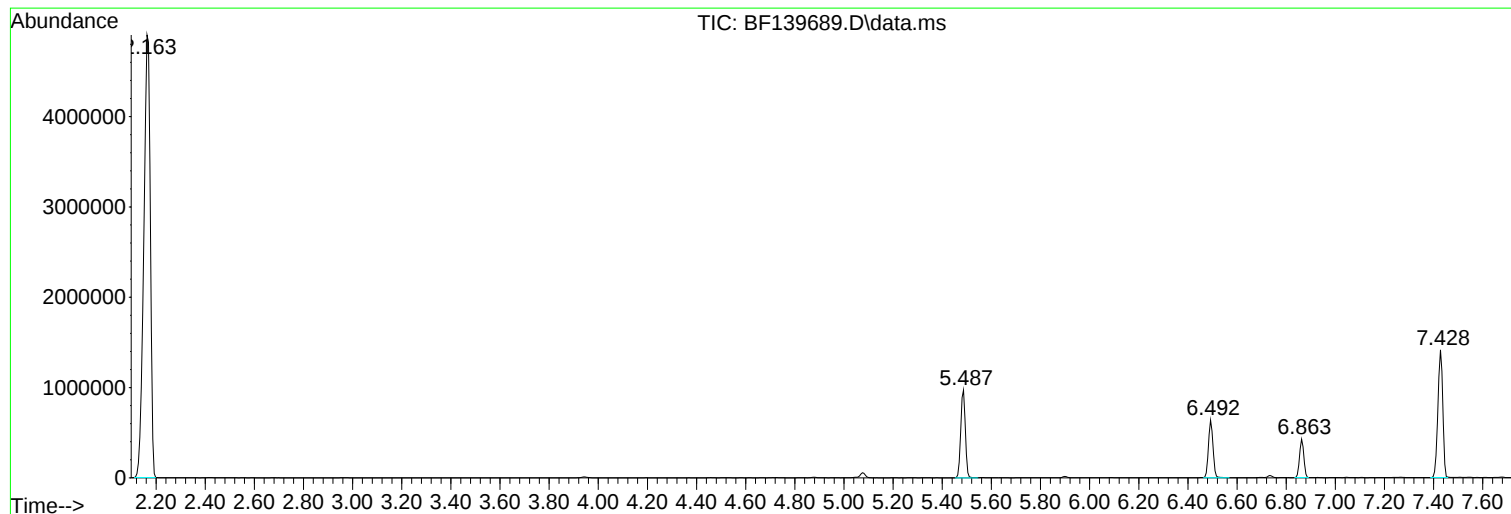
Sum of corrected areas: 25841286

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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
222254

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF100124.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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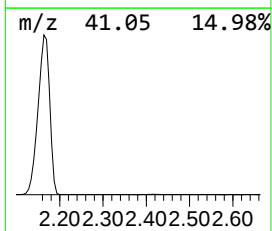
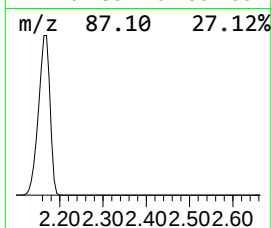
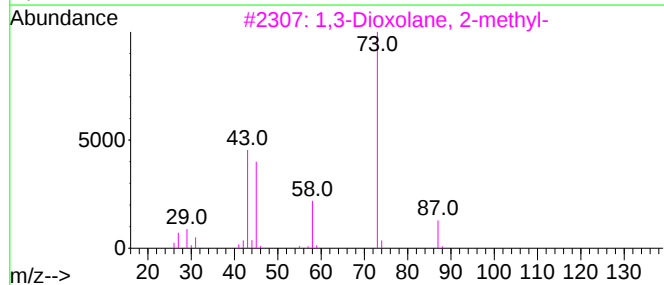
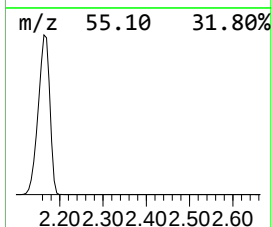
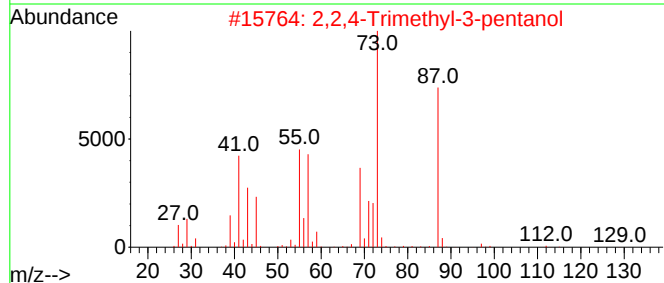
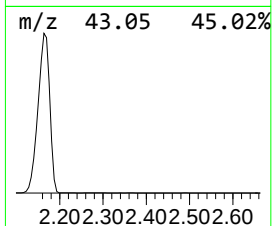
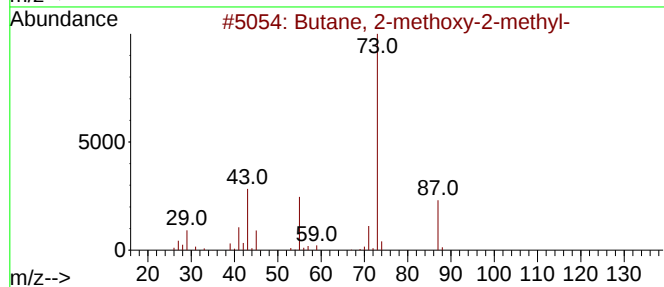
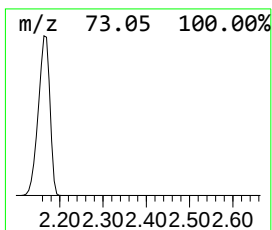
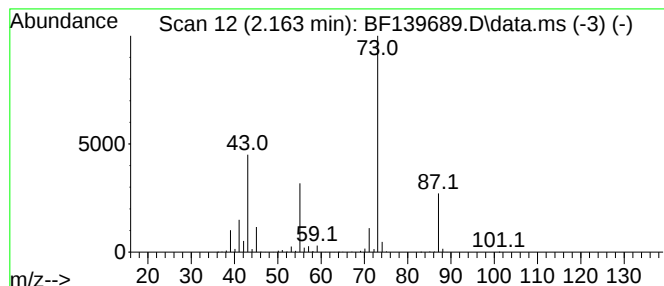
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF100124.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 2.163 | 354.28 ng | 9076270 | 1,4-Dichlorobenzene-d4 | 6.863 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |
| 5    |    |   | N-Ethylformamide            | 73  | C3H7NO  | 000627-45-2 | 9    |



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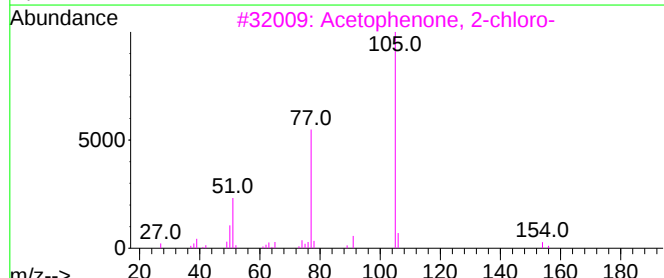
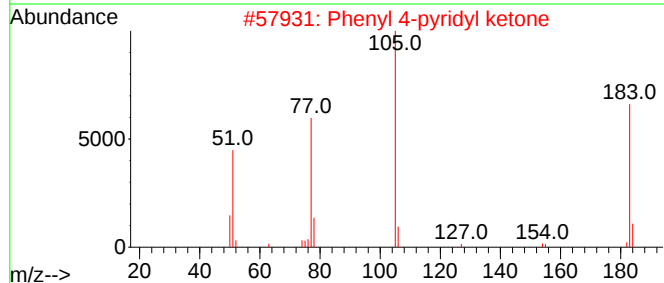
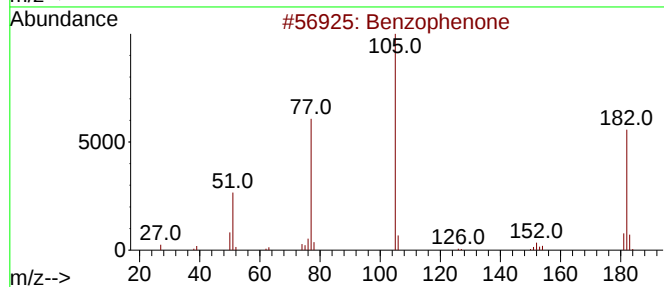
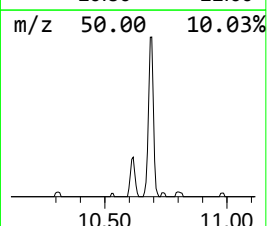
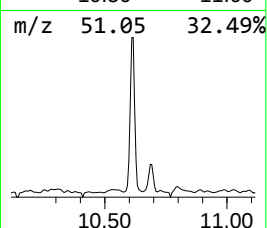
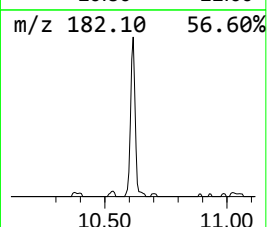
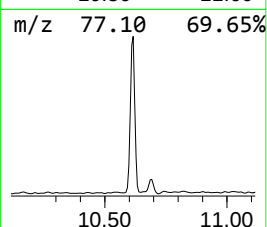
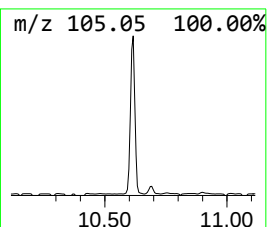
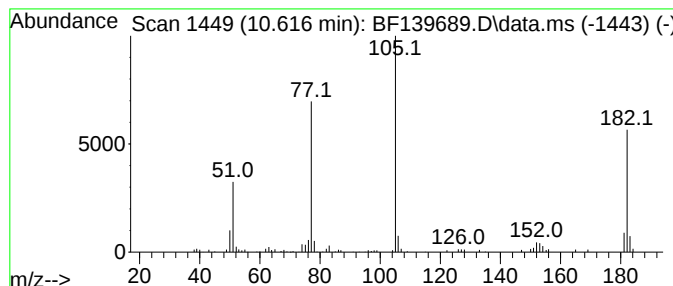
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Benzophenone Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.  |
|--------|---------|-------|------------------|-------|
| 10.616 | 2.41 ng | 92895 | Acenaphthene-d10 | 9.898 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O | 000119-61-9 | 97   |
| 2    |    |   | Phenyl 4-pyridyl ketone             | 183 | C12H9NO | 014548-46-0 | 60   |
| 3    |    |   | Acetophenone, 2-chloro-             | 154 | C8H7ClO | 000532-27-4 | 55   |
| 4    |    |   | Benzoylformic acid                  | 150 | C8H6O3  | 000611-73-4 | 55   |
| 5    |    |   | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS  | 005925-68-8 | 49   |



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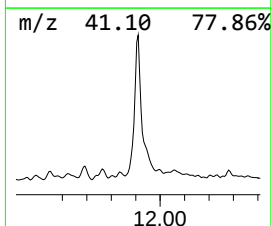
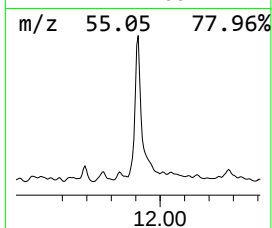
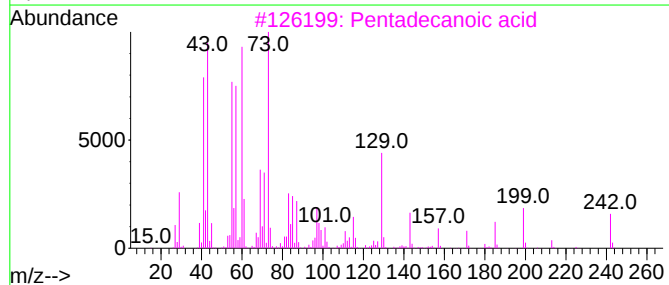
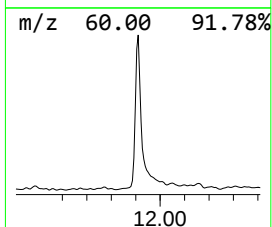
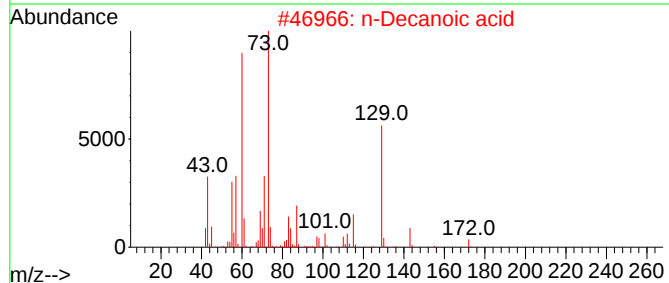
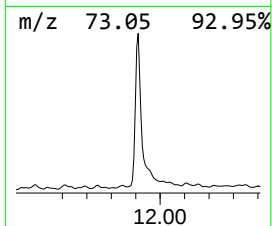
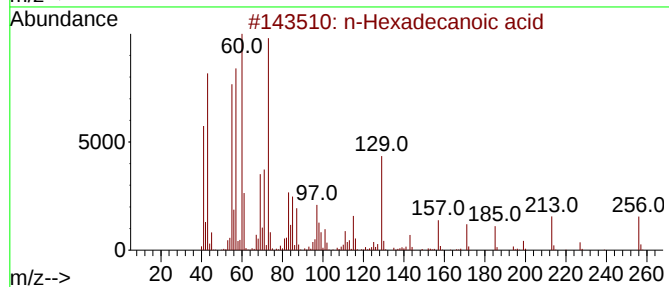
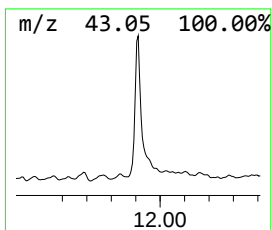
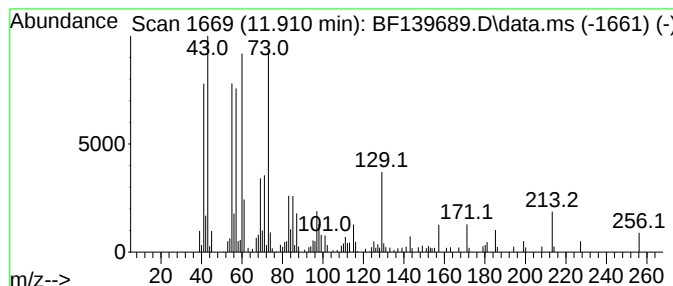
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.910 | 5.12 ng | 214626 | Phenanthrene-d10 | 11.386 |

| Hit# | of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|------|---------------------|-----|----------|-------------|------|
| 1    |      | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |      | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 91   |
| 3    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 5    |      | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 86   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.163  | 354.3   | ng    | 9076270  | 1                     | 6.863  | 512378 | 20.0 |
| Benzophenone       | 10.616 | 2.4     | ng    | 92895    | 3                     | 9.898  | 770921 | 20.0 |
| n-Hexadecanoic ... | 11.910 | 5.1     | ng    | 214626   | 4                     | 11.386 | 838318 | 20.0 |